Redistribution of the Hole Spectral Weight due to Long-Range Spin Correlations in the Three-Band Hubbard Model

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Abstract

In the framework of the three-band model for CuO_2 plane in high-temperature superconductors the spectrum of the spin-polaron hole exitation is investigated. The problem is treated taking into account the coupling of a local polaron with the antiferromagnetic spin wave with $\mathbf{Q} = (\pi, \pi)$.This leads to the essential changes of the lowest polaron band $\epsilon_1(\mathbf{k})$ and the strong redistribution of the bare electron filling.

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In order to understand the nature of high-temperature superconductors it is important to describe properly the motion of a hole in the CuO_2 plane [1, 2]. This motion takes place on the antiferromagnetic (AFM) spin background of copper spins and it must be treated as a correlated motion of a hole coupled to spin excitations (a spin polaron). Usually the spin polaron is studied within the frameworks of the t-J model [1] and the three-band Hubbard model [3, 4, 5]. In the previous works the spin polaron problem was studied mainly in the approximation of a small radius polaron (an analogous of a Zang -Rise polaron). In the present work, for the first time, the long range order of the AFM background is taken into account by introducing an additional new spin polaron of an infinite radius -a bound state of a charge exitation and a spin wave with $\mathbf{Q} = (\pi, \pi)$.We shall show that the introduction of such a

polaron leads to the essential decrease of lowest band filling by bare holes.As a result the area of the Fermi surface strongly increases and its form becomes more complex.

The effective Hamiltonian of the three-band Hubbard model of the CuO_2 plane has the following form in conventional notations [3, 6, 5]:

$$\hat{H} = \hat{T} + \hat{h} + \hat{J}, \qquad \hat{T} = \tau \sum_{\substack{\mathbf{R},\mathbf{a}_1,\mathbf{a}_2,\\ \sigma_1,\sigma_2}} X_{\mathbf{R}}^{\sigma_1\sigma_2} c^{+}_{\mathbf{R}+\mathbf{a}_2,\sigma_2} c_{\mathbf{R}+\mathbf{a}_1,\sigma_1} \tag{1}$$

$$\hat{h} = -h \sum_{\mathbf{R},\mathbf{a},\mathbf{b},\sigma} c^{+}_{\mathbf{R}+\mathbf{a},\sigma} c_{\mathbf{R}+\mathbf{a}+\mathbf{b},\sigma} \ , \qquad \hat{J} = \frac{J}{2} \sum_{\mathbf{R},\mathbf{g}} \hat{\mathbf{S}}_{\mathbf{R}} \hat{\mathbf{S}}_{\mathbf{R}+\mathbf{g}} \ .$$

Here the CuO_2 plane is described by the square sublattice with lattice constant g and two O sites per a Cu unit cell; $\mathbf{R}$ — the vectors of Cu sites, $\mathbf{R}+\mathbf{a}$ — are four vectors of O sites nearest to Cu site $\mathbf{R}$, $\mathbf{a} = \pm\mathbf{a}_x, \pm\mathbf{a}_y$, $\mathbf{a}_x = g(\frac{1}{2}, 0)$, $\mathbf{a}_y = g(0, \frac{1}{2})$. We assume $g = 1$. In (1) we take the notations: $\mathbf{b}$ are the nearest neighbor (NN) vectors for the oxygen sublattice; $\mathbf{g} = 2\mathbf{a}$ and $\mathbf{d} = 2\mathbf{b}$ are the first- and second- NNs for Cu sublattice; the operators c^{+}_{σ} and $X^{\sigma 0}$ create a hole with spin $S = \frac{1}{2}$ and spin projection $\frac{\sigma}{2}$ ($\sigma = \pm 1$) at the O and Cu sites respectively and $X_{\mathbf{R}}^{\sigma_1\sigma_2}$ are the Hubbard projection operators which are convenient for excluding doubly occupied Cu sites.

The first term $\hat{T}$ in (1) describes the effective hole hopping with amplitude from O to O sites through the intervening Cu sites. The term $\hat{J}$ correspond to AFM interaction between Cu sites. $\hat{h}$ represents the direct O–O NN hopping.

Let us discuss the hole excitations with spin $S = \frac{1}{2}$ and the spin projection $\frac{\sigma}{2}$. We shall restrict ourselves to a finite number of site operators $A_{\mathbf{R},j}, (1 \leq j \leq 12)$, in each unit cell $\mathbf{R}$.

In order to treat the hole excitations in the framework of the spin-polaron concept we introduce for each unit cell $\mathbf{R}$ six site operators which describe the local polaron of small radius.

$$A^{+}_{\mathbf{R},\sigma,1(2)} = c^{+}_{\mathbf{R}+\mathbf{a}_x(\mathbf{a}_y),\sigma} \ , \qquad A^{+}_{\mathbf{R},\sigma,3(4)} = \sigma \sum_{\gamma=\pm 1} \gamma X_{\mathbf{R}}^{\overline{\gamma}\,\overline{\sigma}} c^{+}_{\mathbf{R}+\mathbf{a}_x,(\mathbf{a}_y),\,\gamma}$$

$$A^{+}_{\mathbf{R},\sigma,5(6)} = \sigma \sum_{\gamma=\pm 1} \gamma X^{\overline{\gamma}\,\overline{\sigma}}_{\mathbf{R}+\mathbf{g}_x,(\mathbf{g}_y)} c^{+}_{\mathbf{R}+\mathbf{a}_x,(\mathbf{a}_y),\,\gamma} \ , \qquad \overline{\sigma} = -\sigma \tag{2}$$

$$A^{+}_{\mathbf{k},\sigma,j} = \frac{1}{\sqrt{N}} \sum_{\mathbf{R}} \mathrm{e}^{i\mathbf{k}\mathbf{R}} A_{\mathbf{R},\sigma,j} \ .$$

$A^+_{\mathbf{k},\sigma,j}$ are the Fourier transforms of $A^+_{\mathbf{R},\sigma,j}$.

Let us mind, that in our previous investigations [7] this basis of local spin-polaron operators lead to the proper description of the experimentally observed important features of the CuO_2 plane hole spectrum: extended saddle point and isotropic band bottom.

In this paper we want to investigate the role of the delocalized spin polarons which correspond to the coupling of the local polarons to AFM spin wave with momentum $\mathbf{Q} = (\pi, \pi)$, so called Q-polarons usually, if the spin subsystem is found in the state with the AFM long range order then the average value of the amplitude $\langle \mathbf{S_Q} \rangle$ of the spin wave with $\mathbf{q} = \mathbf{Q}$ (the Q-wave) has the macroscopic large value and has the properties analogous to the amplitude of a Bose particle with the zero momentum in the superfluid Bose-gas. As a result for many problems this amplitude can be treated as a $c-$number [8]. Then the coupling of the Q-wave to local electron states does not represent new states but leads, as mentioned above, to the mixing of the states with the momenta $\mathbf{k}$ and $\mathbf{k+Q}$. This treatment is usually based on the widely used Neel type state of the spin subsystem with two sublattices.

But for the S=1/2 spin system the quantum fluctuations are very important and they lead to the spherically symmetric homogeneous Neel state at any small but finite temperature. In this background even at $T = 0$ the average value $\langle \mathbf{S_Q} \rangle = 0$ and the mentioned above simple approach for the hybridization of $\mathbf{k}$ and $\mathbf{k+Q}$ states fails. In the homogeneous Neel state only $\langle \mathbf{S_Q S_Q} \rangle$ can be treated as a macroscopic value. Then the coupling of a local polaron states to $\mathbf{S_Q}$ corresponds to a new delocalized states. In order to take these states into account we introduce the additional six operators based on the basis of (2):

$$A^+_{\mathbf{R},\sigma,j} = \sigma \sum_{\gamma=\pm 1} \gamma Q^{\overline{\gamma}\,\overline{\sigma}}_{\mathbf{R}} A^+_{\mathbf{R},\gamma,i}, \qquad A^+_{\mathbf{k},\sigma,\gamma} = \sigma \sum_{\gamma} \gamma A^+_{\mathbf{k+Q},\gamma,\mathbf{i}} \mathbf{S}^{\overline{\gamma}\,\overline{\sigma}}_{\mathbf{Q}}, \qquad (3)$$

$$Q^{\overline{\gamma}\,\overline{\sigma}}_{\mathbf{R}} \equiv \mathrm{e}^{i\mathbf{QR}} S^{\overline{\gamma}\,\overline{\sigma}}_{\mathbf{Q}} = N^{-1} \sum_{\mathbf{R_1}} e^{i\mathbf{Q}(\mathbf{R}+\mathbf{R_1})} X^{\overline{\gamma}\,\overline{\sigma}}_{\mathbf{R_1}}, \quad j = i+6, \; i = (1 \div 6) \; .$$

In order to determine the spin polaron spectrum $\varepsilon_i(\mathbf{k})$ of 12 quasiparticle bands we use the two time retarded matrix Green's functions $G_{i,j}(t, \mathbf{k})$ for the operators $A_{\mathbf{k},\sigma,i}$:

$$G_{i,j}(t, \mathbf{k}) \equiv \left\langle A_{\mathbf{k},i}(t) | A^+_{\mathbf{k},j}(0) \right\rangle = -i\Theta(t) \left\langle \left\{ A_{\mathbf{k},i}(t) \; , A^+_{\mathbf{k},j}(0) \right\} \right\rangle \; , \qquad (4)$$

We solve the system of the equations of motion for $G_{i,j}(\omega, \mathbf{k})$ by using the standard Mori-Zwanzig projection technique and restricting ourselves to the above chosen basis of operators $\{A_{\mathbf{k},\sigma,i}\}$ (2,3). Then the Green's functions and the spectrum are determined from the equations:

$$\left(\omega - DK^{-1}\right) G = K\,, \quad det|K\varepsilon(\mathbf{k}) - D| = 0. \tag{5}$$

$$D_{i,j}(\mathbf{k}) = \left\langle \left\{ B_{\mathbf{k},i}\,, A^{+}_{\mathbf{k},l} \right\} \right\rangle, \quad K_{i,j} = \left\langle \left\{ A_{\mathbf{k},i}\,, A^{+}_{\mathbf{k},j} \right\} \right\rangle\,, \quad B_{\mathbf{k},i} = \left[A_{\mathbf{k},i}\,, H \right]\,. \tag{6}$$

The matrix elements of D and K are expressed both through short-range spin-correlation functions of Cu subsystem and the long-range order correlation function $\langle \mathbf{S_Q S_Q} \rangle$. The Cu spin subsystem is described by the $S = \frac{1}{2}$ Heisenberg model at $T = 0$. For the value of the correlation functions we use the results of [9] where this model was treated in the framework of spherically symmetrical Green's functions theory. It is important that we take into account that $\langle\, bf S_{\mathbf{Q}} \mathbf{S_Q} \rangle$ is a macroscopic value and is equal to a square of effective sublattice magnetization:

$$\langle \mathbf{S_Q S_Q} \rangle = \lim_{\mathbf{R_1} \to \infty} |\langle \mathbf{S_R S_{R+R_1}} \rangle| = M^2 \tag{7}$$

Note that the dependence of the spin polaron excitations spectrum on the long-range correlation function $\langle \mathbf{S_Q S_Q} \rangle$ appears only due to treatment of the Q-polaron states (3). Below we take the following numerical values of the spin-correlation functions: $\langle \mathbf{S_R S_{R+g}} \rangle = -0.3521$, $\langle \mathbf{S_R S_{R+d}} \rangle = 0.229$, $\langle \mathbf{S_R S_{R+2g}} \rangle = 0.2$, $M^2 = 0.0914$. The matrix elements were calculated in the low hole doping limit, $n << 1$, n -is the total number of oxygen holes per unit cell. The detailed expressions of matrices D and K will be published elsewhere.

As a result the Green's functions have a form

$$G_{i,j}(\omega, \mathbf{k}) = \sum_{l=1}^{12} \frac{Z^{(l)}_{(i,j)}(\mathbf{k})}{\omega - \varepsilon_l(\mathbf{k})}. \tag{8}$$

In particular the value of $Z_h(\mathbf{k}) = Z^{(1)}_{(1,1)}(\mathbf{k}) + Z^{(1)}_{(2,2)}(\mathbf{k})$ corresponds to the number of bare oxygen holes with the fixed spin σ and the momentum $\mathbf{k}$ in the state $|\mathbf{k}, \sigma\rangle$ of the lowest quasiparticle band $\varepsilon_1(\mathbf{k})$. Let us mind that residue $Z_{(i,j)}(\mathbf{k})$ satisfy the sum rule $\sum_s Z^{(s)}_{(i,i)}(\mathbf{k}) = \mathbf{1}, \mathbf{i} = \mathbf{1}, \mathbf{2}$.This means

that in this model the Luttinger theorem is not fulfilled and the maximum number of holes per cell is equal four despite the presents of twelve bands.

The results of the most interesting two lowest bands $\varepsilon_1(\mathbf{k})$ and $\varepsilon_2(\mathbf{k})$ for realistic values of model parameters $J_1 = 0.2\tau$, $h = 0.4\tau$ (below all energetical parameters are expressed in units τ) are presented in Fig.1(a). In the same figure the spectrum of the lowest of six bands $\underline{\varepsilon}_1(\mathbf{k})$, calculated in the approximation of six operators (2) is shown. In Fig.1(b) the spectrum $\varepsilon_1(\mathbf{k})$ is presented by the equal-energy lines $\varepsilon_1(\mathbf{k}) = \text{const}$. Let us mind that the Q-polarons may lead to a rather complex form of the Fermi surface.This circumstance can give a nontrivial behaviour of the Hall effect on doping, and even cause the inversion of the Hall constant if the Fermi energy is close to $\varepsilon_1(\mathbf{k}) = -\mathbf{4.5}$.

As it is seen from Fig.1(a), the inclusion of the Q-wave qualitatively leads to the decoupling of the lowest band of the local small polaron excitations and $\varepsilon_1(\mathbf{k})$ is close to $\underline{\varepsilon}_1(\mathbf{k})$. This means that the main features of the lowest band excitations previously calculated in the local polaron approximation [7] are preserved.

The importance of the treatment of the Q-wave polarons may be seen if we discuss the filling of the lowest band by bare holes. In Fig.1(c) the filling of the $\varepsilon_1(\mathbf{k})$ and $\underline{\varepsilon}_1(\mathbf{k})$ are shown, i.e., the residues $Z_h(\mathbf{k})$ and $\underline{Z}_h(\mathbf{k})$ (the underlined values correspond to local polaron approximation). One can see that the introduction of the Q-polarons leads to the essential decrease of hole filling along the lines X-M and M-N.This redistribution of the bare hole spectrum weight explaines the results of photoemission experiments when the"flat band region" is observed along the direction X-Γ and is invisible along the line X-M. Fig.1(d) demonstrates that the local polaron concept(six operators (2)) leads to the strong decrease of the filling under the Fermi surface. This means the violation of the Luttinger theorem approximately in four times (the analogous effect was found in [10]).But the inclusion of a Q-polaron states (3) leads to the addition essential reduction of filling, approximately in 1.5 times.The maximum $\varepsilon_1(\mathbf{k})$ -band filling is equal to $n = 0.22$, and the smallness of this value justifies our low density approximation.

Formula (3) points out that the Q-polaron $A^+_{\mathbf{k},\sigma,\mathbf{7(8)}}$ contains a bare hole state $c^+_{\mathbf{k}+\mathbf{Q},\sigma}$. It means that the residual $Z_{\mathbf{Q}}$ of the corresponding Green's function $G_{\mathbf{Q}}(\mathbf{k}) = \mathbf{G_{7,7}} + \mathbf{G_{8,8}}$ are responsible for "shadow band" effect [11].

We are to note that Q-polaron scenario reproduces the essential decrease

of the lowest band width with the decrease of the AFM constant J. Usually such an effect is obtained only in the self-consistent Born approximation [12].

In conclusion we want to mention that the described above properties of the spin polaron are mainly preserved if we suppose that the spin subsystem has no long range order, but the spin correlation length L is large. Then, in the matrix elements of D and K we must replace the long-range correlation function $\langle S_{\mathbf{Q}} S_{\mathbf{Q}} \rangle$ by the following expression:

$$\sum_{|\mathbf{q}|<\delta q} \langle S_{\mathbf{Q}+\mathbf{q}} S_{\mathbf{Q}+\mathbf{q}} \rangle \qquad \delta q \approx 1/L, \; L >> 1. \tag{9}$$

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Figure caption

Fig.1: (a) The spectra $\varepsilon_1(\mathbf{k})$ and $\varepsilon_2(\mathbf{k})$ calculated for the basis (2),(3), and the spectrum $\underline{\varepsilon}_1(\mathbf{k})$ calculated for the basis (2). The spectra are given along symmetrical lines $\Gamma - X - M - N - \Gamma$ and $X - N - X$; $\Gamma = (0,0)$; $X = (\pi,0),(0,\pi)$, $M = (\pi,\pi)$; $N = (\pi/2,\pi/2)$;

(b) Spectrum equal-energy lines $\varepsilon_1(\mathbf{k}) = const$;

(c) $Z_h(\mathbf{k})$ and $\underline{Z}_h(\mathbf{k})$ — the number of bare holes (the residues of corresponding Green's functions) in the quasiparticle excitations for the spectra $\varepsilon_1(\mathbf{k})$ and $\underline{\varepsilon}_1(\mathbf{k})$; $Z_Q(\mathbf{k})$ is the residue of the lowest pole $\varepsilon_1(\mathbf{k})$; for the Green's function $G_{11,11}(\omega,\mathbf{k}) + G_{12,12}(\omega,\mathbf{k})$, which characterize the "shadow band" effect;

(d) the dependence of the number of holes n per unit cell on the value of the Fermi surface area S (S_{BZ} – the area of the first Brillouine zone): thick line — for the spectrum $\varepsilon_1(\mathbf{k})$; dashed line — for the spectrum $\underline{\varepsilon}_1(\mathbf{k})$; solid straight line — the case of the noninteracting particle filling.

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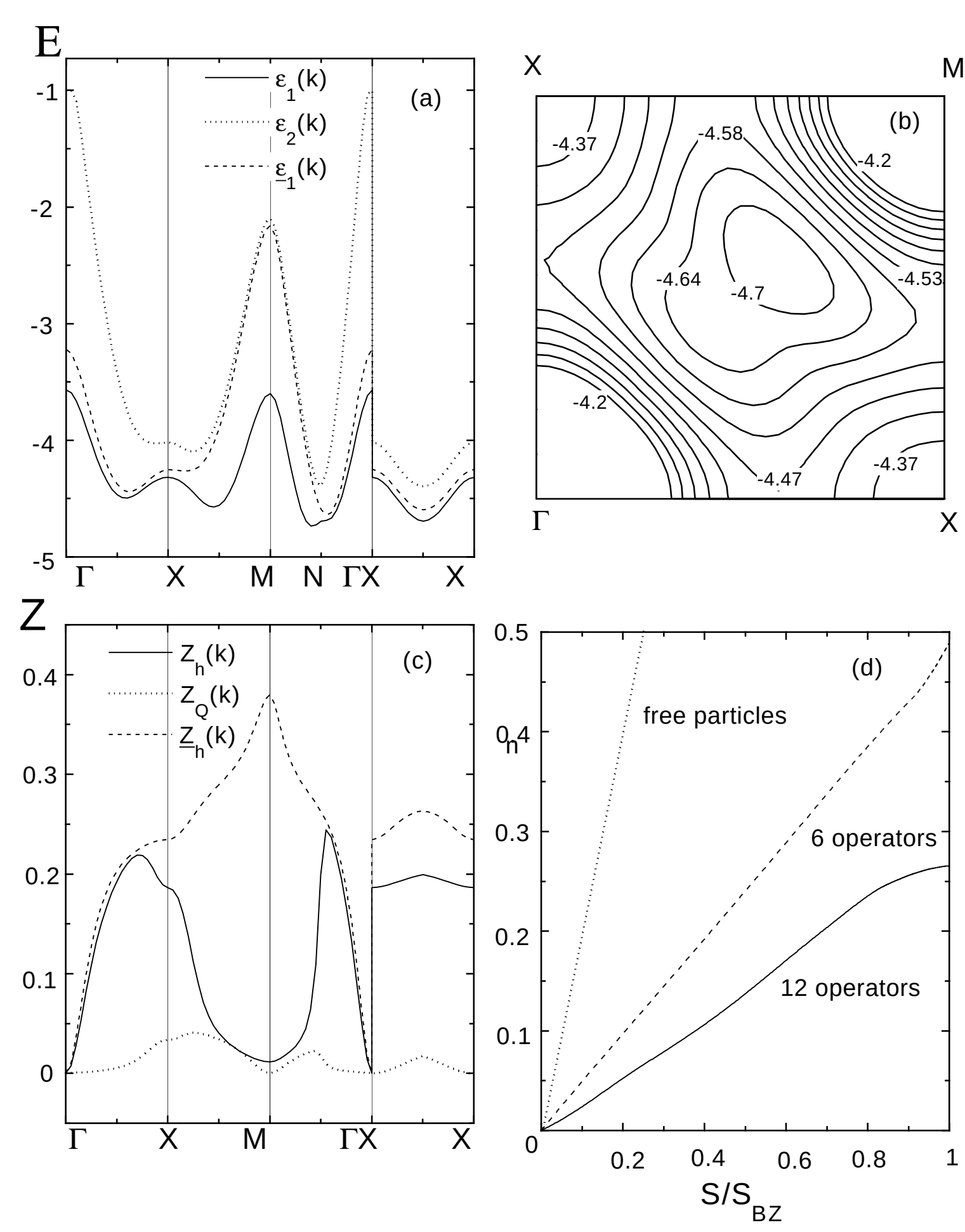
E
ε1(k)
ε2(k)
ε−1(k)
(a)
-1
-2
-3
-4
-5
Γ
X
M
N
ΓX
X
X
M
(b)
-4.37
-4.58
-4.2
-4.64
-4.7
-4.53
-4.2
-4.47
-4.37
Γ
X
Z
Zh(k)
ZQ(k)
Z−h(k)
(c)
0.4
0.3
0.2
0.1
0
Γ
X
M
ΓX
X
0.5
0.4
0.3
0.2
0.1
0
n
(d)
free particles
6 operators
12 operators
0
0.2
0.4
0.6
0.8
1
S/SBZ